

Triethanolamine
102-71-6 | DTXSID9021392

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.01

Global applicability domain: Inside

Local applicability domain index: 4.68e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Triethanolamine</div> <div>Measured: -1.00</div> <div>Predicted: -1.01</div>	<div>Image not found</div> <div>Diethanolamine</div> <div>Measured: -1.43</div> <div>Predicted: -1.46</div>	<div>Image not found</div> <div>Diethyl L-tartrate</div> <div>Measured: -0.290</div> <div>Predicted: -0.481</div>
<div>Image not found</div> <div>Triethylene glycol</div> <div>Measured: -1.75</div> <div>Predicted: -1.33</div>		